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Bulk heterojunction photovoltaic cells based on Merocyanine dye aggregates

Solution-processed bulk-heterojunction (BHJ) devices based on lowmolecular-weight organic dyes are an emerging research field with high potential for cost-effective generation of electricity from solar light. Until to date, only few dyes could be identified as suitable electron donor components with high power conversion efficiencies of >5%. Our recent observation that dipolar merocyanine dyes, which are widely applied as nonlinear optical and photorefractive materials, exhibit such remarkable photovoltaic properties motivates us to explore innovative strategies of solutionprocessing such as supramolecular polymerization and dye aggregation and to elucidate the impact on dye aggregation on molecular and materials properties by experimental and theoretical means. Thus, the major objective in the forthcoming project period is on the synthesis of new tailored bis- and trismerocyanine dyes forming bimolecular complexes and zipper-type ladder structures with a defined □-stacking arrangement of dipolar merocyanine dyes and to investigate their optical, redox and photovoltaic properties. Furthermore, quantum chemical calculations will be performed to gain a deeper insight into the impact of dye aggregation on charge and exciton transport properties of these dye aggregates as well as crystalline merocyanine derivatives.